Methyl-d1 radical, oxo-
24286-05-3 | DTXSID90179017

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 2.70 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.92e-01

Confidence level: 6.93e-01

Nearest Neighbors from the Training Set

Image not found
Methanol
Measured: 2.75
Predicted: 2.76

Image not found
Ethyleneimine
Measured: 6.03
Predicted: 4.17

Image not found
Ethanol
Measured: 1.58
Predicted: 2.24

Image not found
Acetic acid
Measured: 1.00
Predicted: 2.40

Image not found
Acetamide
Measured: 5.01
Predicted: 4.44